

ON THE APPROXIMATION OF CONTRACTIVE SEMIGROUPS OF OPERATORS IN DISCRETIZABLE HILBERT SPACES

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Dedicated to the memory of professor Salvador Llopis.

ABSTRACT. The Computation of discrete Contractive semigroups becomes necessary when we deal with several types of evolution equations in Discretizable Hilbert spaces, in this work we study some properties of the discrete forms of the contractive semigroups induced by an approximation scheme in a prescribed Hilbert space, we also deal with the implementation of computational methods in this Hilbert Space and apply some of the results presented here in the Heisenberg representation of quantum dynamical semigroups.

1. INTRODUCTION

In this article we will work with evolution equations defined on a Hilbert space $H := H^n(G)$ that have the form:

$$\begin{cases} u'(t) = Au(t) + f(t) \\ u(0) = u_0 \end{cases} \quad (1.1)$$

with $A \in \mathcal{L}(H)$ constant in time and with $\operatorname{Re} \sigma(A) \leq 0$ and where $u_0 \in H$. In (1.1) we have that the operator A represents in some suitable sense the spatial differential and boundary condition operators.

The set $\{s_t : t \in \mathbb{T} \subseteq \mathbb{R}\}$ is called a contractive semigroup generated by A if we have that $\lim_{h \rightarrow 0^+} h^{-1}(s_h - \mathbf{1}) = A$ and also

S1: $s_t s_v = s_{t+v}$, $t, s \in \mathbb{T}$ and $s_0 = \mathbf{1}$;

S2: $\|s_t\|_{\mathcal{L}(H)} \leq 1$, $t \in \mathbb{T}$;

S3: $s_t x \in C(\mathbb{T}, H) \cap C^1(\mathbb{T}, H)$, $t \in \mathbb{T}$.

In the following sections we will present the abstract setup needed to perform the computation of the discrete semigroups of operators and the corresponding numerical analysis of the behavior of its elements, also we will apply the results here presented to the Heisenberg representation of quantum dynamical semigroups.

2. DISCRETIZATION SCHEMES

2.1. Discretizable Hilbert Spaces. In general we will have that a discretizable Hilbert space $H(G)$, with $G \subset \mathbb{R}^N$ compact, will be considered as any linear space that is both a separable and a reproducing kernel Hilbert space. One of the basic

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elements that we will use to perform the general discretization process is the grid that will be defined as follows.

Definition 2.1. *Grid:* For two given sets $G \subseteq \mathbb{R}^N$ and $\mathbb{G} = \{0, \dots, M_m\} \subseteq \mathbb{Z}$, with M_m a number that depends on a fixed number m , a fixed value $h \in \mathbb{R}^N$ and a bijection $f : \mathbb{Z} \rightarrow \mathbb{R}^N : \mathbb{G} \ni k \mapsto g \in \mathbb{R}^N$, the set $G_{m,h} = \{g_k \in G : g_k = f(k), k \in \mathbb{G}\}$ is called a grid in G of size h and length M_m or simply a grid.

For a given discretizable Hilbert space $H(G)$ one can define an operator $P_{m,h} \in \mathcal{L}(H)$ called particular projector and defined in the following way.

Definition 2.2. *Particular Projector:* An operator $P_{m,h} \in \mathcal{L}(H)$, with H a discretizable hilbert space, that satisfies the relations:

$$P_{m,h}^2 = P_{m,h} \quad (2.1)$$

$$P_{m,h}x \xrightarrow{h \rightarrow 0^+} x \quad (2.2)$$

$$\|P_{m,h} - \mathbf{1}\|_* \leq c_* h^{\mu_m} \quad (2.3)$$

will be called a particular projector, in (2.3) $\|\cdot\|_*$ represents any prescribed norm in $\mathcal{L}(H)$ and μ_m is a number that depends on m that will be called projection order with respect to $\|\cdot\|_*$.

For a given particular projector $P_{m,h}$ in a discretizable Hilbert space $H(G)$ we will denote by $H_{m,h}$ its corresponding subspace. A particular projector $P_{m,h}$ can be factored in the form:

$$P_{m,h} = p_{m,h} p_{m,h}^\dagger \quad (2.4)$$

where the operators $p_{m,h}^\dagger \in \mathcal{L}(H, H^*)$ and $p_{m,h} \in \mathcal{L}(H^*, H)$ are called decomposition and expansion factors of $P_{m,h}$ respectively. For each $m \in \mathbb{Z}^+$ a particular projector $P_{m,h} \in \mathcal{L}(H)$ is related to a basis $\mathcal{P} = \{p_1, \dots, p_{N_m}\} \subseteq H$ through the following expression:

$$P_{m,h} p_k = p_k, \forall p_k \in \mathcal{P} \quad (2.5)$$

also we will have that each $p_k \in \mathcal{P}$ will satisfy prescribed conditions $Bp_k = P_k^b, x \in \partial G$ that are compatible with the boundary value conditions of the problem described by (1.1) in some suitable sense, and that the decomposition factor $p_{m,h}^\dagger$ in (2.4) is determined by a prescribed grid $G_{m,h} \subseteq G$ through the relation:

$$p_{m,h}^\dagger x = \hat{x} = \{c_k(x, G_{m,h})\}, k \in \mathbb{G} = \{1, \dots, N_m\}. \quad (2.6)$$

For a given discretizable Hilbert space H whose inner product is induced by the inner product map $\mathcal{M} \in \mathcal{L}(H, H^*)$ in the following way

$$\langle x, y \rangle_H := \mathcal{M}[x](y) \quad (2.7)$$

one can define a particular representation given by

$$\mathcal{M}_{m,h}p_{m,h}^\dagger \cdot := \mathcal{M}P_{m,h} \cdot \quad (2.8)$$

that will receive the name of inner product matrix form relative to $H_{m,h} := P_{m,h}H$, it can be seen that

$$\begin{aligned}\langle x, y \rangle_{H_{m,h}} &= \mathcal{M}_{m,h}[p_{m,h}^\dagger x](p_{m,h}^\dagger y) \\ &= [p_{m,h}^\dagger y]^* \mathcal{M}_{m,h}[p_{m,h}^\dagger x] \\ &= \mathcal{M}[P_{m,h}x](P_{m,h}y) \\ &= \langle P_{m,h}x, P_{m,h}y \rangle_H\end{aligned}$$

from this relations we can obtain the following results.

Theorem 2.1. *Every inner product matrix form is symmetric and positive definite (SPD).*

Proof. It can be seen that for a discretizable Hilbert space H and a given particular projector $P_{m,h}$ in H , with basis $\mathcal{P} = \{p_1, \dots, p_{N_m}\}$, we will have that

$$\begin{aligned}(\mathcal{M}_{m,h})_{i,j} &= \mathcal{M}_{m,h}[p_{m,h}^\dagger p_i](p_{m,h}^\dagger p_j) \\ &= \langle P_{m,h}p_i, P_{m,h}p_j \rangle_H \\ &= \langle p_i, p_j \rangle_H \\ &= \overline{\langle p_j, p_i \rangle_H} \\ &= \overline{\langle P_{m,h}p_j, P_{m,h}p_i \rangle_H} \\ &= \mathcal{M}_{m,h}[p_{m,h}^\dagger p_j](p_{m,h}^\dagger p_i) \\ &= \overline{(\mathcal{M}_{m,h})_{j,i}}\end{aligned}$$

and this implies that $\mathcal{M}_{m,h} = \mathcal{M}_{m,h}^*$. Now since

$$0 \leq \|x\|_{H_{m,h}}^2 = \langle x, x \rangle_{H_{m,h}} = \mathcal{M}_{m,h}p_{m,h}^\dagger x$$

we will have that $\mathcal{M}_{m,h}x > 0$ for each $0 \neq x \in H \setminus \text{Ker } P_{m,h}$. \square

Corollary 2.1. *Every inner product matrix form is invertible.*

2.2. Discretization of Operators. Using particular projectors one can obtain for a given operator $B \in \mathcal{L}(H)$ a corresponding representation defined by the following definition.

Definition 2.3. *Particular Representation of an Operator. For a given operator $B \in \mathcal{L}(X, Y)$ being X, Y discretizable Hilbert spaces and being $X_{m,h}, Y_{m,h}$ the subspaces relative to the particular projectors $P_{m,h} \in \mathcal{L}(X), Q_{m,h} \in \mathcal{L}(Y)$, the operator $B_{m,h} \in \mathcal{L}(X_{m,h}^*, Y_{m,h}^*)$ given by*

$$B_{m,h} := q_{m,h}^\dagger B p_{m,h} \tag{2.9}$$

will be called particular representation of B .

Once we have computed the particular representation of a given operator $B \in \mathcal{L}(X, Y)$ over a discretizable Hilbert spaces X, Y , in prescribed subspaces $X_{m,h} \leq X, Y_{m,h} \leq Y$ determined by a particular projectors $P_{m,h}, Q_{m,h}$, we will define the approximation order of a particular representation as follows.

Definition 2.4. *Approximation order of a particular representation.* We say that the particular representation $B_{m,h} \in \mathcal{L}(X_{m,h}^*, Y_{m,h}^*)$ of an operator $B \in \mathcal{L}(X, Y)$ is of order ν_m (with ν_m a value that depends of the prescribed number m) with respect to a given norm $\|\cdot\|_*$ in Y if for each $x \in X$ there exists c_* that does not depend on h such that:

$$\left\| B_{m,h} p_{m,h}^\dagger x - q_{m,h}^\dagger Bx \right\|_* \leq c_* h^{\nu_m} \quad (2.10)$$

3. SOBOLEV CHAINS AND PARTICULAR FACTORIZATION

3.1. Sobolev Chain. If for a given Discretizable Hilbert space $X_0 := X^n(G)$ and a prescribed sequence of operators in $\mathcal{L}(X_0)$ $\mathcal{B} := \{b_k\}_{k=0}^n$ we can define a sequence of Hilbert spaces of the form $\mathcal{X} := \{X_k\}_{k=0}^n$, that satisfy the relation:

$$X_0 := b_0 X, X_{k+1} := b_{k+1} X_k, 0 \leq k \leq n-1 \quad (3.1)$$

the Hilbert space

$$Y_n := \bigoplus_{0 \leq k \leq n} X_k \quad (3.2)$$

equipped with the inner product

$$\langle x, y \rangle_{Y_n} = \sum_{0 \leq k \leq n} \langle x_k, y_k \rangle_{X_k} \quad (3.3)$$

$$= \sum_{0 \leq k \leq n} \langle B_k x_0, B_k y_0 \rangle_{X_k} = \langle x_0, y_0 \rangle_{Y_n} \quad (3.4)$$

with B_k defined by

$$B_k := \prod_{0 \leq j \leq k} b_j \quad (3.5)$$

the pair \mathcal{X}, \mathcal{B} described above will be called a Sobolev chain based on X_0 and generated by \mathcal{B} .

3.2. Particular Factorization of Operators. Sobolev chains are particularly useful when we are working with operators over a prescribed discretizable Hilbert space X , in this work a particularly important kind of chains will be those chains that permit us to write an operator $A \in \mathcal{L}(X)$ in the following way

$$A = aa^\dagger \quad (3.6)$$

in this cases we can easily obtain a particular factorization of A using the Sobolev chain $\{X_0, X_1\}, \{\mathbf{1}, a^\dagger\}$ that will have the form

$$\mathcal{A}_{m,h}\cdot := [p_{m,h}^\dagger \cdot]^* \mathcal{A}_{m,h}[p_{m,h}^\dagger \cdot] \quad (3.7)$$

$$= \mathcal{M}_{m,h}a_{m,h}^\dagger \cdot \quad (3.8)$$

$$= [p_{m,h}^\dagger \cdot]^* (a_{m,h}^\dagger)^* \mathcal{M}_{m,h}(a_{m,h}^\dagger)[p_{m,h}^\dagger \cdot] \quad (3.9)$$

$$= \left\langle a_{m,h}^\dagger p_{m,h}^\dagger x, a_{m,h}^\dagger p_{m,h}^\dagger x \right\rangle_{X_0} \quad (3.10)$$

$$= \langle P_{m,h} \cdot, P_{m,h} \cdot \rangle_{X_1} \quad (3.11)$$

the expression presented in (3.7) will be called particular pactorization of A , the graphic form of the particular factorization of $A \in \mathcal{L}(X)$ and its relation to $A \in$

$\mathcal{L}(X)$ itself and to this particular type of Sobolev chain, can be expressed by the following diagram

$$\begin{array}{ccccc}
 X_{1,m,h}^* & \xleftarrow{(a_{m,h}^\dagger)^*} & X_{0,m,h} & \xrightarrow{a_{m,h}^\dagger} & X_{1,m,h} \\
 \mathcal{M}_{m,h} \downarrow & & \downarrow \mathcal{A}_{m,h} & \searrow A_{m,h} & \downarrow a_{m,h} \\
 X_{1,m,h}^* & \xrightarrow{a_{m,h}^\dagger} & X_{2,m,h}^* & \xrightarrow{\mathcal{M}_{m,h}^{-1}} & X_{2,m,h}
 \end{array}$$

from (3.7) and (3.9) we obtain the following results.

Theorem 3.1. *For a given Sobolev chain $\{X_0, X_1\}$, $\{\mathbf{1}, a^\dagger\}$ the matrix $\mathcal{A}_{m,h}$ is symmetric and positive definite.*

Proof. It can be seen that

$$\begin{aligned}
 \mathcal{A}_{m,h}^* &= ((a_{m,h}^\dagger)^* \mathcal{M}_{m,h} (a_{m,h}^\dagger))^* \\
 &= (a_{m,h}^\dagger)^* \mathcal{M}_{m,h}^* (a_{m,h}^\dagger) \\
 &= (a_{m,h}^\dagger)^* \mathcal{M}_{m,h} (a_{m,h}^\dagger) \\
 &= \mathcal{A}_{m,h}
 \end{aligned}$$

also we may check that

$$\begin{aligned}
 [p_{m,h}^\dagger x]^* \mathcal{A}_{m,h} [p_{m,h}^\dagger x] &= \langle P_{m,h} x, P_{m,h} x \rangle_{X_1} \\
 &= \|P_{m,h} x\|_{X_0}^2 \geq 0
 \end{aligned} \tag{3.12}$$

then for $0 \neq x \in X_0 \setminus (Ker P_{m,h} \cap Ker a_{m,h}^\dagger)$ we will have that $[p_{m,h}^\dagger x]^* \mathcal{A}_{m,h} [p_{m,h}^\dagger x] > 0$.

□

In this point we are going to present a very useful property of an operator that will be defined by.

Definition 3.1. *For a given Hilbert space X , an operator $B \in \mathcal{L}(X)$ is said to be accretive if for any $x \in X$ we have that*

$$Re \langle Bx, x \rangle_X \geq 0 \tag{3.13}$$

From T.3.1 we can obtain the following.

Corollary 3.1. *For a given Sobolev chain $\{X_0, X_1\}$, $\{\mathbf{1}, a^\dagger\}$ the particular representation $A_{m,h} = \mathcal{M}_{m,h}^{-1} \mathcal{A}_{m,h}$ of $A = aa^\dagger$ is accretive.*

And using this corollary and T.A.3 it is not very difficult to see that.

Corollary 3.2. *For a given Sobolev chain $\{X_0, X_1\}$, $\{\mathbf{1}, a^\dagger\}$ the particular representation $A_{m,h} = \mathcal{M}_{m,h}^{-1} \mathcal{A}_{m,h}$ of $A = -aa^\dagger$ satisfies the condition $Re \sigma(A_{m,h}) \leq 0$.*

4. DISCRETIZATION OF SEMIGROUPS

As a part of the process of studying the numerical solution to (1.1), we start with the discretization of the semigroups induced by $A \in \mathcal{L}(H)$, with this in mind we obtain some results that will be presented below.

If we denote by $\{s_t : t \in \mathbb{T}\}$ the semigroup generated by $A \in \mathcal{L}(H)$, then the discrete representation of it will be denoted by $\{\tilde{s}_k : k \in \mathbb{K}\}$, with $\mathbb{K} \subseteq \mathbb{Z}_0^+$, discrete semigroups mimic some of the properties of the continuum ones in the following way:

DS1: $\tilde{s}_k \tilde{s}_j = \tilde{s}_{k+j}, k, j \in \mathbb{K}$ and $\tilde{s}_0 = \mathbf{1}$;

DS2: $\|\tilde{s}_k\|_{\mathcal{L}(H_{m,h})} \leq 1, k \in \mathbb{K}$.

as in the first section, we will have that the elements of the discrete semigroup will be related to the particular representation $A_{m,h} \in \mathcal{L}(H_{m,h}^*)$ of $A \in \mathcal{L}(H)$ through the expression $\lim_{\tau \rightarrow 0^+} \tau^{-1}(\tilde{s}_1 - \mathbf{1}) = A$.

4.1. Polynomial time discretization of semigroups. If we rewrite the equation (1.1) using the particular representation of its spatial part we obtain the following abstract semidiscrete initial value problem

$$u'_{m,h}(t) = A_{m,h}u_{m,h}(t) + f_{m,h}(t) \quad (4.1)$$

with initial condition $u_{m,h}(0) = \hat{u}_0 = P_{m,h}u_0$, whose exact solution can be computed using the time continuous semigroup $\{\hat{g}_t : t \in \mathbb{T}\}$, with $\hat{g}_t := e^{tA_{m,h}}$, in the following way:

$$u_{m,h}(t) = \hat{g}_t u_{m,h}(0) + \int_0^t \hat{g}_{t-s} f(s) ds \quad (4.2)$$

if we can take an abstract Taylor polynomial of n -th order around $t = 0$ of the solution to (1.1) when $f(t) = 0$, we obtain

$$u_\tau := \sum_{k=0}^n \frac{1}{k!} (\tau A)^k u_0 = \tilde{g}_\tau u_0 \quad (4.3)$$

here \tilde{g}_τ is called basic element of the discrete semigroup of n -th order relative to $A \in \mathcal{L}(A)$, because of the following relation

$$\{\tilde{s}_{n,k} : \tilde{s}_{n,k} := \tilde{g}_\tau^k, k \in \mathbb{K}\} \quad (4.4)$$

it is not very difficult to see that for a given polynomial integration scheme that is exact for n -th order polynomials described by

$$\mathcal{Q}_n v := \sum_{j=0}^n w_j v(j\tau) \quad (4.5)$$

one can obtain a better approximation $\hat{s}_{n\tau} u_0$ to the solution of (1.1) with respect to a given initial estimation in the following way

$$\hat{s}_{n\tau} \hat{u}_0 = [\mathcal{Q}_n A \tilde{s}_{n,\cdot}] \hat{u}_0 + \mathcal{Q}_n \tilde{s}_{n,n-\cdot} f(\cdot). \quad (4.6)$$

4.2. Semigroups generated by particular representations. When we have a discrete semigroup $\{\tilde{s}_{n,k} : \tilde{s}_{n,k} := \tilde{g}_\tau^k, k \in \mathbb{K}\}$ where \tilde{g}_τ is defined in the same way as in (4.3), and we also have that $\lim_{\tau \rightarrow 0^+} \tau^{-1}(\tilde{s}_{n,1} - \mathbf{1}) = A_{m,h}$ with $A_{m,h} \in \mathcal{L}(X_{m,h}^*)$ being the particular representation of an operator $A \in \mathcal{L}(X)$, with X a discretizable Hilbert space, we say that the discrete semigroup is generated by $A_{m,h}$, the polynomial that represents \tilde{g}_τ in this case will be described by

$$\tilde{g}_\tau := \sum_{k=0}^n \frac{1}{k!} (\tau A_{m,h})^k. \quad (4.7)$$

4.3. Stability and Convergence. In this section we will consider that for m, h fixed a given particular representation $A_{m,h} \in \mathbb{C}^{N_m \times N_m}$, of a prescribed accretive operator $A \in \mathcal{L}(X)$ is related to a particular projector $P_{m,h}$, with basis $\mathcal{P} = \{p_k\}_{k=0}^{N_m}$ in a discretizable Hilbert space X , and also that (4.7) can be expressed in the form

$$\tilde{g}_\tau = \sum_{k=0}^n \frac{1}{k!} (P_A^{-1} \tau D_A P_A)^k \quad (4.8)$$

$$= \sum_{k=0}^n \frac{1}{k!} P_A^{-1} \tau^k D_A^k P_A \quad (4.9)$$

where $D_A \in \mathbb{C}^{N_m \times N_m}$ is a diagonal matrix defined by

$$D_A := \text{diag}\{\lambda_j\} = \begin{pmatrix} \lambda_0 & 0 & \cdots & 0 & 0 \\ 0 & \lambda_1 & & & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & & & \lambda_{N_m-1} & 0 \\ 0 & 0 & \cdots & 0 & \lambda_{N_m} \end{pmatrix} \quad (4.10)$$

with $\lambda_j \in \sigma(A_{m,h})$, $j \in \{1, \dots, N_m\}$, and where $P_A \in \mathbb{C}^{N_m \times N_m}$ is defined by

$$P_A := \begin{pmatrix} v_1 & v_2 & \cdots & v_{N_m} \end{pmatrix} \quad (4.11)$$

with $A_{m,h} v_j = \lambda_j v_j$, $j \in \{0, \dots, N_m\}$, which means that the j -th column of P_A is the eigenvector that corresponds to the j -th eigenvalue of $A_{m,h}$. If $A \in \mathcal{L}(X)$ can be factored using a Sobolev chain of the form $\{X_k\}_{k=0,1,a}$, with $X_0 = X$, then from (3.9) we will have that

$$A_{m,h} = (a_{m,h}^\dagger)^* \mathcal{M}_{m,h} (a_{m,h}^\dagger) \quad (4.12)$$

and this implies that

$$\tilde{g}_\tau = \sum_{k=0}^n \frac{1}{k!} P_A^* \tau^k D_A^k P_A \quad (4.13)$$

from T.A.3, T.A.6 in appendix A and T.B.1 in appendix B we get the following results concerning to stability of the approximation schemes.

Theorem 4.1. Stability 1. *If an operator $A \in \mathcal{L}(X)$ can be factored using a Sobolev chain of the form $\{X_0, X_1\}, \{\mathbf{1}, a^\dagger\}$ with $X_0 = X$ a discretizable Hilbert space, then the basic element \tilde{g}_τ of the discrete semigroup generated by $-A \in \mathcal{L}(X)$ and described in (4.13) will satisfy the relation*

$$\|\tilde{g}_\tau\|_{\mathcal{L}(X_{m,h})} = \left\| \mathcal{M}_{m,h}^{1/2} \tilde{g}_\tau \mathcal{M}_{m,h}^{-1/2} \right\|_2 \leq 1 \quad (4.14)$$

when $\tau = \alpha h^d / K_A$, with $\|\hat{A}_{m,h}\|_\infty \leq K_A h^{-d}$, $\hat{A}_{m,h} = \mathcal{M}_{m,h}^{1/2} A_{m,h} \mathcal{M}_{m,h}^{-1/2}$ and $0 < \alpha \leq 1$.

Proof. From corollary C.A.1 we will have that $\|\hat{A}_{m,h}\|_2 \leq \|\hat{A}_{m,h}\|_\infty$ and clearly $\tau = \alpha h^d / K_A \leq \|\hat{A}_{m,h}\|_\infty^{-1} \leq \|\hat{A}_{m,h}\|_2^{-1}$. Now since $\tilde{g}_\tau = \hat{P}_A^* p_n(\tau \hat{D}_A) \hat{P}_A$ with

$$p_n(z) := \sum_{k=0}^n \frac{1}{k!} z^k \quad (4.15)$$

and if we represent by $\mu \in \mathbb{R}$ and $\kappa \in \mathbb{R}$ the values $\mu := \sup\{|\lambda| : \lambda \in \sigma(\hat{A}_{m,h})\}$ and $\kappa := \inf\{|\lambda| : \lambda \in \sigma(\hat{A}_{m,h})\}$ we will have that

$$\begin{aligned} \|\hat{P}_A^* p_n(\tau \hat{D}_A) \hat{P}_A\|_2 &= \|\hat{P}_A^* p_n(\alpha h^d / K_A \hat{D}_A) \hat{P}_A\|_2 \\ &\leq \|\hat{P}_A^* p_n(\mu^{-1} \hat{D}_A) \hat{P}_A\|_2 \\ &\leq p_n\left(\alpha \frac{\kappa}{\mu}\right) \\ &\leq 1 \end{aligned}$$

□

From the last result we can easily obtain the following

Corollary 4.1. *Stability 2. If an operator $A \in \mathcal{L}(X)$ can be factored using a Sobolev chain of the form $\{X_0, X_1\}, \{\mathbf{1}, a^\dagger\}$ with $X_0 = X$ a discretizable Hilbert space, then the basic element \tilde{g}_τ of the discrete semigroup generated by $-A \in \mathcal{L}(X)$ and described in (4.13) will satisfy the relation*

$$\|\tilde{g}^k\|_{\mathcal{L}(X_{m,h})} \leq 1, \quad k \geq 0. \quad (4.16)$$

Also for any given $k \geq 0$ it can be seen that

Theorem 4.2. *Cauchy condition. If $k \geq 0$ then $\|\tilde{u}((k+1)\tau) - \tilde{u}(k\tau)\|_{X_{m,h}} \leq \tilde{c}_1 v^k$ where v is a value ≤ 1 .*

Proof. Since $\tilde{u}(j\tau) = \tilde{s}_{n,j} \hat{u}_0$ we will have that

$$\begin{aligned} \|\tilde{u}((k+j)\tau) - \tilde{u}(k\tau)\|_{X_{m,h}} &= \|(\tilde{s}_{n,k+j} - \tilde{s}_{n,k}) \hat{u}_0\|_{X_{m,h}} \\ &= \|\tilde{s}_{n,k} (\tilde{s}_{n,j} - \mathbf{1}) \hat{u}_0\|_{X_{m,h}} \\ &\leq \|\tilde{g}_\tau^k\|_{\mathcal{L}(X_{m,h})} \|\tilde{g}_\tau^j - \mathbf{1}\|_{\mathcal{L}(X_{m,h})} \|\hat{u}_0\|_{X_{m,h}} \\ &\leq \|p(\tau A_{m,h})\|_{\mathcal{L}(X_{m,h})}^k \|q(\tau A_{m,h})\|_{\mathcal{L}(X_{m,h})} \|\hat{u}_0\|_{X_{m,h}} \\ &\leq \left(p\left(\frac{\kappa}{\mu}\right)\right)^k |q(1)| \|\hat{u}_0\|_{X_{m,h}} \end{aligned}$$

with $p(z) := \sum_{k=0}^n \frac{1}{k!} z^k$, $q(z) := (p(z))^j - 1$, $\mu := \sup\{|\lambda| : \lambda \in \sigma(A_{m,h})\}$ and $\kappa := \inf\{|\lambda| : \lambda \in \sigma(A_{m,h})\}$, taking $v = p(\kappa/\mu)$ and $\tilde{c}_1 = |q(1)| \|\hat{u}_0\|_{X_{m,h}}$ concludes the proof. □

Concerning to convergence of the approximation schemes we can obtain the following result.

Theorem 4.3. Convergence. *If for a given accretive operator $B \in \mathcal{L}(X)$ and each $x \in X$ we have that $e^{k\tau A_{m,h}}$, $k\tau \in \mathbb{T}$, with $A = -B$, has approximation order ν_m with respect $\|\cdot\|_X$ and if there exists $K_A \in \mathbb{R}_0^+$ such that we can take $\tau := \alpha h^d / K_A$ with $K_A h^{-d} \geq \|A_{m,h}\|_\infty$ and with $1 \geq \alpha := h^{\frac{\nu_m}{n+1}}$, where $n \in \mathbb{Z}_0^+$ is a prescribed number, then we will have that there exists a constant C_2 such that*

$$\left\| p_{m,h}^\dagger u(k\tau) - \tilde{s}_{n,k} p_{m,h}^\dagger u(0) \right\|_X \leq C_2 h^{\nu_m}.$$

Proof. Here we will consider that $e^{k\tau A_{m,h}}$ has approximation order ν_m with respect to $\|\cdot\|_X$ wich implies

$$\begin{aligned} \|\hat{u}(k\tau) - \tilde{s}_{n,k} \hat{u}_0\|_{X_{m,h}} &\leq \|\hat{u}(k\tau) - e^{k\tau A_{m,h}} \hat{u}_0\|_{X_{m,h}} + \\ &\quad \|e^{k\tau A_{m,h}} \hat{u}_0 - \tilde{s}_{n,k} \hat{u}_0\|_{X_{m,h}} \\ &\leq c_2 h^{\nu_m} + \left\| \sum_{j=n+1}^{\infty} \frac{r_j}{j!} (k\tau A_{m,h})^j \hat{u}_0 \right\|_{X_{m,h}} \\ &\leq c_2 h^{\nu_m} + \left\| \frac{r_{n+1}}{(n+1)!} k^{n+1} \tau^{n+1} A_{m,h}^{n+1} \right\|_{\mathcal{L}(X_{m,h})} \|\hat{u}_0\|_{X_{m,h}} \\ &\leq c_2 h^{\nu_m} + \\ &\quad \frac{r_{n+1}}{(n+1)!} h^{\nu_m} k^{n+1} \left\| \left(\frac{h^d}{K_A} A_{m,h} \right)^{n+1} \right\|_{\mathcal{L}(X_{m,h})} \|\hat{u}_0\|_{X_{m,h}} \\ &\leq c_2 h^{\nu_m} + \frac{r_{n+1}}{(n+1)!} k^{n+1} h^{\nu_m} \|\hat{u}_0\|_{X_{m,h}} \\ &= \left(c_2 + \frac{r_{n+1}}{(n+1)!} k^{n+1} \|\hat{u}_0\|_{X_{m,h}} \right) h^{\nu_m} \end{aligned}$$

here $r_k := 1 - k!C(\{b_j\}, k)$ where $C(\{b_j\}, k)$ are the multinomial coefficients that correspond to the coefficients $\{b_j\}$ of the abstract polynomial $\tilde{s}_{n,k}$, taking $C_2 = c_2 + \frac{k^{n+1} r_{n+1}}{(n+1)!} \|\hat{u}_0\|_{X_{m,h}}$ concludes the proof. \square

5. APPLICATION TO EVOLUTION OF OPERATORS IN THE HEISENBERG PICTURE

In this section we will describe a basic procedure of implementation of the results presented in this work in the computation of evolution of observables of a quantum system in the Heisenberg picture, here we will consider that all the quantum systems are modeled in a discretizable Hilbert space X with inner product $\langle u, v \rangle_X$ given by

$$\langle u, v \rangle_{X(G)} := \int_G u \bar{v} d\mu(G). \quad (5.1)$$

where $d\mu(G)$ is the volume mesure element in G , also we will consider that we can take a particular projector $P_{m,h} \in \mathcal{L}(X, X_{m,h})$ compatible prescribed boundary value condtions in some suitable sense and whose decomposition and expansion factors are related to a prescribed grid $G_{m,h} \subset G$ and basis $\mathcal{P} := \{p_k\}$ respectively.

5.1. Quantum Dynamical Semigroups. For a given quantum system on a discretizable Hilbert space $X := X^2(G)$ whose wave function $\psi \in C([0, T], X^2(G)) \cap C^1([0, T], X^2(G))$ is modeled by a Schrödinger equation of the form

$$E\psi(t) = H\psi(t) \quad (5.2)$$

here $\mathcal{L}(X^n(G)) \ni H := pp^\dagger, p^\dagger \longrightarrow -\frac{i}{\hbar}\nabla + \beta$, with $\nabla := \hat{e}_k \sum_k \partial_k$ and $E \longrightarrow \frac{i}{\hbar}\partial_t$. If (5.2) has initial value $\psi(0) = \psi_0 \in X$ and is subject to boundary value conditions of the form $B_H\psi = \psi_b, x \in \partial G$.

If we take a scale where $\hbar = 1$, we can obtain a particular representation of H denoted by $H_{m,h}$, using this representation (5.2) will take the form

$$\begin{cases} \hat{\psi}'(t) = -iH_{m,h}\hat{\psi}(t) \\ \hat{\psi}(0) = \hat{\psi}_0 \end{cases} \quad (5.3)$$

the n -th order semigroup $\{U_{n,k} : U_{n,k} := G_\tau^k, k \in \mathbb{K}\}$ generated by $-iH_{m,h}$ will be called n -th order quantum dynamical semigroup in the Schrödinger representation where $G_\tau := \sum_{k=0}^n \frac{1}{k!}(-i\tau H_{m,h})$, using the elements of this semigroup we can write the solution to (5.2) in the form

$$\hat{\psi}(k\tau) = U_{n,k}\hat{\psi}_0. \quad (5.4)$$

When we work with particular representations of equations like (5.3) we will have as an application of T.4.1 that:

Theorem 5.1. *Stability of Complex Semigroups. If an operator $A \in \mathcal{L}(X)$ can be particularly factored using a Sobolev chain of the form $\{X_0, X_1\}, \{\mathbf{1}, a^\dagger\}$ with $X_0 = X$ a discretizable Hilbert space, then the basic element of the \tilde{G}_τ of the discrete semigroup generated by $-A \in \mathcal{L}(X)$ and described by*

$$\tilde{G}_\tau := \sum_{k=0}^n \frac{1}{k!}(i\tau A_{m,h}), \mathbb{Z}_0^+ \ni n \geq 1 \quad (5.5)$$

will satisfy the relation

$$\|\tilde{G}_\tau\|_{\mathcal{L}(X_{m,h})} = \|\mathcal{M}_{m,h}^{1/2}\tilde{G}_\tau\mathcal{M}_{m,h}^{-1/2}\|_2 \leq 1 \quad (5.6)$$

when $\tau = \alpha h^d/K_A$, with $\|\hat{A}_{m,h}\|_\infty \leq K_A h^{-d}$, $\hat{A}_{m,h} = \mathcal{M}_{m,h}^{1/2}A_{m,h}\mathcal{M}_{m,h}^{-1/2}$ and $0 < \alpha \leq 1$.

Proof. Since $A_{m,h}$ is accretive we will have that $\hat{A}_{m,h}$ will be accretive too and from C.A.1 we will have that $\|\hat{A}_{m,h}\|_2 \leq \|\hat{A}_{m,h}\|_\infty$ and clearly $\tau = \alpha h^d/K_A \leq \|\hat{A}_{m,h}\|_\infty^{-1} \leq \|\hat{A}_{m,h}\|_2^{-1}$. Now since $\tilde{G}_\tau = \hat{P}_A^* p_m(i\tau \hat{D}_A) \hat{P}_A$ with

$$p_n(z) := \sum_{k=0}^n \frac{1}{k!} z^k \quad (5.7)$$

and if we represent by $\mu \in \mathbb{R}$ and $\kappa \in \mathbb{R}$ the values $\mu := \sup\{|\lambda| : \lambda \in \sigma(\hat{A}_{m,h})\}$ and $\kappa := \inf\{|\lambda| : \lambda \in \sigma(\hat{A}_{m,h})\}$ we will have that

$$\begin{aligned} \|\hat{P}_A^* p_m(i\tau \hat{D}_A) \hat{P}_A\|_2 &= \|\hat{P}_A^* p_m(i\alpha h^d/K_A \hat{D}_A) \hat{P}_A\|_2 \\ &\leq \|\hat{P}_A^* p_m(i\mu^{-1} \hat{D}_A) \hat{P}_A\|_2 \\ &\leq \left| p_n\left(i\alpha \frac{\kappa}{\mu}\right) \right| \\ &\leq 1 \quad . \end{aligned}$$

□

Following a similar procedure to the followed in the proves of T.4.3 and T.5.1 we can obtain the following result.

Theorem 5.2. *Convergence of complex semigroups. If for a given observable (symmetric operator) $A \in \mathcal{L}(X)$ and for each $x \in X$ we have that $e^{ik\tau A_{m,h}}$, $k\tau \in \mathbb{T}$ has approximation order ν_m with respect $\|\cdot\|_X$ and if there exists $K_A \in \mathbb{R}_0^+$ such that we can take $\tau := \alpha h^d / K_A$ with $K_A h^{-d} \geq \|A_{m,h}\|_\infty$ and with $1 \geq \alpha := h^{\frac{\nu_m}{n+1}}$, where $n \in \mathbb{Z}_0^+$ is a prescribed number, then we will have that there exists a constant C_3 such that*

$$\left\| p_{m,h}^\dagger u(k\tau) - \tilde{s}_{n,k} p_{m,h}^\dagger u(0) \right\|_X \leq C_3 h^{\nu_m}$$

where $\tilde{s}_{n,k} := \tilde{G}_\tau^k$ with $\tilde{G}_\tau := \sum_{k=0}^n \frac{1}{k!} (i\tau A_{m,h})^k$.

Proof. Here we will consider that $e^{ik\tau A_{m,h}}$ has approximation order ν_m with respect to $\|\cdot\|_X$ and that the value $\mu_{m,h} := \sup\{\|\lambda\| : \lambda \in \sigma(\mathcal{M}_{m,h}^{1/2} A_{m,h} \mathcal{M}_{m,h}^{-1/2})\}$ wich implies

$$\begin{aligned} \|\hat{u}(k\tau) - \tilde{s}_{n,k} \hat{u}_0\|_{X_{m,h}} &\leq \|\hat{u}(k\tau) - e^{ik\tau A_{m,h}} \hat{u}_0\|_{X_{m,h}} + \\ &\quad \|e^{ik\tau A_{m,h}} \hat{u}_0 - \tilde{s}_{n,k} \hat{u}_0\|_{X_{m,h}} \\ &\leq c_3 h^{\nu_m} + \left\| \sum_{j=n+1}^{\infty} \frac{r_j}{j!} (ik\tau A_{m,h})^j \hat{u}_0 \right\|_{X_{m,h}} \\ &\leq c_3 h^{\nu_m} + k^{n+1} h^{\nu_m} \left| Q_{n+1} \left(i \frac{h^d}{K_A} \mu_{m,h} \right) \right| \|\hat{u}_0\|_{X_{m,h}} \\ &\leq c_3 h^{\nu_m} + \frac{r_{n+1}}{(n+1)!} k^{n+1} h^{\nu_m} \|\hat{u}_0\|_{X_{m,h}} \\ &= \left(c_3 + \frac{r_{n+1}}{(n+1)!} k^{n+1} \|\hat{u}_0\|_{X_{m,h}} \right) h^{\nu_m} \end{aligned}$$

here $Q_{n+1}(z)$ is defined by

$$Q_{n+1}(z) := \frac{r_{n+1}}{(n+1)!} z^{n+1} \left(\sum_{k=0}^{\infty} q_k z^k \right)^{1/2} \quad (5.8)$$

with $r_{n+1} := 1 - (n+1)! C(\{a_j\}, n+1)$, $q_0 := 1$, $q_j := \frac{1-j! C(\{a_j\}, n+1)}{r_{n+1}}$, $j \geq 1$ and where $C(\{a_j\}, n+1)$ are the multinomial coefficients corresponding to the coefficients $\{a_j\}$ of the abstract polynomial $\tilde{s}_{n,k}$, taking $C_3 = c_3 + \frac{k^{n+1} r_{n+1}}{(n+1)!} \|\hat{u}_0\|_{X_{m,h}}$ concludes the proof. \square

Now, for any given observable $B \in \mathcal{L}(X)$ with particular representation given by $B_{m,h} \in \mathcal{L}(X_{m,h}^*)$ (operator) we can obtain its Heisenberg evolution through the computation

$$\hat{B}_{n,k} := U_{m,k}^\dagger B_{m,h} U_{n,k} \quad (5.9)$$

the set $\{\hat{B}_{n,j} : \hat{B}_{n,j} = U_{n,j}^\dagger B U_{n,k}\}$ will be called quantum dynamical semigroup in the Heisenberg representation, also we can compute its expected value that will be described by

$$\mathbb{E}(\hat{B}_{n,k}) := \left\langle \hat{B}_{n,k} \right\rangle = \left\| U_{n,k} \hat{\psi}_0 \right\|_{X_{m,h}}^{-2} \left\langle B_t \hat{\psi}_0, \hat{\psi}_0 \right\rangle_{X_{m,h}}. \quad (5.10)$$

5.2. Computation of Quantum Dynamical Semigroups in the Heisenberg representation. In this section we will present an example of numerical computation of a quantum dynamical semigroup in the Heisenberg representation and more specifically the Heisenberg evolution of the position operator $\mathbf{X} \in \mathcal{L}(X)$ a prescribed quantum system.

Example 5.1. *For the quantum system consisting of a particle in a bidimensional box represented by $G = [-1, 1]^2$ and whose wave function is modeled by the Schrödinger equation*

$$\begin{cases} \partial_t \psi = -iH\psi, & x \in G \\ \psi(0) = \psi_0 \\ \psi = 0, & x \in \partial G \end{cases} \quad (5.11)$$

here $H := pp^\dagger$ with $p^\dagger = -i[\partial_x, \partial_y]$, for this example we will use the Sobolev chain $\{X_0, X_1\}, \{\mathbf{1}, p^\dagger\}$, also we will have that

$$\langle u, v \rangle_X := \int_G u \bar{v} dx dy \quad (5.12)$$

and $G_{m,h} := \{x_{j_k}\} \times \{x_{j_k}\}$, where $\{x_j\}$ the Gauss-Lobatto grid of order 2, $\mathcal{B} := \{\ell_{i_k} \otimes \ell_{j_k}\}$, ℓ_{i_k} the i_k -th cardinal basis (Lagrange interpolating system) with respect to $\{x_{j_k}\}$, wich means that $\ell_{j_k}(x_{i_k}) = \delta_{j_k, i_k}$, with $\delta_{i,j}$ the Kronecker delta, using the particular factorization of $-iH_{2,1/8}$ we can obtain the particular decomposition of the spatial part of (5.11) in the following way

$$\hat{\psi}'(t) = -iH_{2,1/8}\hat{\psi}(t) \quad (5.13)$$

with $H_{2,1/8} = \mathcal{M}_{2,1/8}^{-1}[p_{2,1/8}^\dagger]^* \mathcal{M}_{2,1/8}[p_{2,1/8}^\dagger]$, in this particular case we have that:

$$\mathcal{M}_{2,1/8} := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \mathcal{W}_{2,1/8}(w) \quad (5.14)$$

with $\mathcal{W}_{2,1/8}(w) := \text{diag}\{w_{j_k}\}$ an operator that depends in a suitable sense on the basic integrating matrix $w \in \mathbb{R}^{3 \times 3}$ of second order defined by

$$w := \begin{pmatrix} 1/3 & 0 & 0 \\ 0 & 4/3 & 0 \\ 0 & 0 & 1/3 \end{pmatrix} \quad (5.15)$$

and also we will have that

$$p_{2,1/8}^\dagger := i \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \mathcal{W}_{2,1/8}^{-1/2}(w) \begin{bmatrix} D_{2,1/8}(d) \otimes \mathbf{1} \\ \mathbf{1} \otimes D_{2,1/8}(d) \end{bmatrix} \quad (5.16)$$

where $D_{2,1/8}(d) \in \mathcal{L}(X_{2,1/8}^*)$ is an operator that depends in some suitable sense on the basic differentiation matrix $d \in \mathbb{R}^{3 \times 3}$ of approximation order 2 for the Gauss-Lobatto spectral element method wich is defined by:

$$d := \begin{pmatrix} -3/2 & 2 & -1/2 \\ -1/2 & 0 & 1/2 \\ 1/2 & -2 & 3/2 \end{pmatrix} \quad (5.17)$$

now, since spectral methods of this kind have approximation order $m+2$ with respect to $\|\cdot\|_{X_{m,h}}$, we can take $\alpha = 1/8$ and $\tau = (1/16)^3 \|d^2\|_\infty^{-1}$, using $H_{2,1/8}$ we can

compute the basic element of the discrete semigroup $\{U_{3,k} : U_{3,k} = \hat{G}_\tau^k\}$ that will be defined in the form

$$\hat{G}_\tau := 1 - i\tau H_{2,1/8} - \frac{(\tau H_{2,1/8})^2}{2} + \frac{i(\tau H_{2,1/8})^3}{6} \quad (5.18)$$

using the elements of the discrete semigroup we can compute $\hat{\mathbf{X}}_{3,k}$ in the form:

$$\hat{\mathbf{X}}_{3,k} := \hat{U}_{3,k}^* \hat{\mathbf{X}} \hat{U}_{3,k} \quad (5.19)$$

and its expected value $\langle \hat{\mathbf{X}}_{3,k} \rangle$ can be computed using the expression:

$$\langle \hat{\mathbf{X}}_{3,k} \rangle := (\mathbb{E}(x_{2,1/8}), \mathbb{E}(y_{2,1/8})) \quad (5.20)$$

with

$$\mathbb{E}(\cdot) = \frac{1}{\mathcal{P}_\psi} \hat{\psi}_0^* \hat{U}_{3,k}^* \mathcal{M}_{2,1/8}(\cdot) \hat{U}_{3,k} \hat{\psi}_0 \quad (5.21)$$

and where

$$\mathcal{P}_\psi := \hat{\psi}_0^* \hat{U}_{3,k}^* \mathcal{M}_{2,1/8} \hat{U}_{3,k} \hat{\psi}_0. \quad (5.22)$$

now, since the particular factorization $\mathcal{H}_{2,1/8} := \mathcal{M}_{2,1/8} H_{2,1/8}$ of $H \in \mathcal{L}(X)$ is clearly symmetric by T.3.1 for the value of τ used in this example we can use theorems T.5.1 and T.5.2 presented above to predict the behavior of the evolution operators in the discrete semigroup relative to this quantum system.

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APPENDIX A. SOME THEOREMS FROM LINEAR ALGEBRA

In this section we will present some basic theorems from linear algebra that are very useful in the study of some processes and methods presented in this work.

Theorem A.1. *Any symmetric positive/negative definite matrix is invertible.*

Theorem A.2. *For a given matrix $\mathbf{A} \in \mathbb{C}^{m \times n}$ we will have that*

$$\|\mathbf{A}\|_{\infty} := \max_i \sum_j |\mathbf{A}_{i,j}|.$$

Theorem A.3. *Every symmetric positive/negative definite matrix $\mathbf{A} \in \mathbb{C}^{m \times n}$ has all of its eigenvalues real positive/negative and its eigenvectors form an orthogonal system.*

Theorem A.4. *For a given matrix $\mathbf{A} \in \mathbb{C}^{m \times n}$ we will have that*

$$\|\mathbf{A}\|_2 := \max\{\sqrt{\lambda} : \lambda \in \sigma(\mathbf{A}^* \mathbf{A})\}.$$

Theorem A.5. *Gershgorin Theorem. For any given matrix $\mathbf{A} \in \mathbb{C}^{m \times n}$ we will have that $\sigma(\mathbf{A}) \subset \bigcup_i D_i$ with*

$$D_i := \{z \in \mathbb{C} : |z - \mathbf{A}_{i,i}| \leq \sum_{j \neq i} |\mathbf{A}_{i,j}|\}, 1 \leq i \leq m$$

Using theorems T.A.5 and T.A.3 one can obtain the following.

Corollary A.1. *For any symmetric positive/negative definite/semi-definite matrix $\mathbf{A} \in \mathbb{C}^{m \times n}$ we will have that*

$$\|\mathbf{A}\|_2 \leq \|\mathbf{A}\|_\infty.$$

Theorem A.6. *For any given matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$ and any $\lambda \in \sigma(\mathbf{A})$ whose corresponding eigenvector is given by $v_\lambda \in \mathbb{C}^n$ we will have for every polynomial $p_m(z) := a_0 + a_1 z + \dots + a_m z^m \in \mathcal{P}_m(\mathbb{C})$, with $\mathcal{P}_m(\mathbb{C})$ the set of all polynomials of degree $\leq m$, that $p_m(\lambda) \in \sigma(p_m(\mathbf{A}))$ will be an eigenvalue of $p_m(\mathbf{A}) \in \mathbb{C}^{n \times n}$ with corresponding eigenvector $v_\lambda \in \mathbb{C}^n$.*

APPENDIX B. A THEOREM FROM REAL ANALYSIS.

In this section we will present a basic theorem from real analysis that is very useful in the study of some processes presented in this article.

Theorem B.1. *Let $\sum a_n$ be a number series such that*

$$\lim_{n \rightarrow \infty} a_n = 0$$

such that the terms a_n are alternating positive and negative and such that $|a_{n+1}| \leq |a_n|$ for $n \geq 0$. Then the series converge and

$$\left| \sum_{n=0}^{\infty} a_n \right| \leq |a_0|. \quad (\text{B.1})$$

Remark B.1. *From the last theorem we also have*

$$\left| \sum_{n=k}^{\infty} a_n \right| \leq |a_k| \quad (\text{B.2})$$

and

$$\left| \sum_{n=k}^m a_n \right| \leq |a_k|. \quad (\text{B.3})$$

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